**Undergraduate women empowering women in computational chemistry: three perspectives**

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**Abstract**

The undergraduate computational chemistry research group headed by Mauricio Cafiero at Rhodes College has a history of including, promoting and supporting women in this predominantly male field. Alums of this research group from 2004 to 2019 include 9 M.D.s, 2 science researchers, 2 Ph.D.s, 1 secondary teacher, 2 pharmacists, a physical therapist, 2 nurses, 6 current medical school students and 5 current science graduate students. They have produced 18 peer reviewed publications with female undergraduate first authors and over 100 conference presentations, including 9 international conference presentations. While Professor Cafiero does all he can to support these students, he attributes the continuous success of the group at recruiting, retaining and supporting these women to the students themselves. The students' success and visibility on campus helps to recruit new students; the heavy presence of women in this group provides a strong support system for women who may otherwise feel isolated in a male-dominated field; and these support groups provide models and support for women to overcome common obstacles that women in science face. We will profile three recent graduates who will discuss how the above points affected them during their time in the research group and discuss their experience in the context of some literature on women in STEM.

## 1. Introduction

We would like to discuss the composition of and structures and relationships in our computational chemistry lab at Rhodes College in reference to the research that exists on undergraduate women in STEM, undergraduate women in undergraduate research and undergraduate students in research overall. An emphasis of this work will be on the strong lineage of women in the group for the past 15 years, and how these women have been empowered by those that preceded them and how they in turn empower those that came after. Finally, we will present our suggestions for best practices in recruiting and retaining women in computational chemistry. The research advisor is a Latino male with a PhD in theoretical and computational chemistry from the University of Arizona. He served as an NRC post-doc at the National Institute of Standards and Technology and has been at Rhodes college since 2004 where he has earned the title of Professor and served for three years as the Director of Fellowships and Undergraduate Research. The three student authors (all graduated in 2019) are Rebecca Evans, who graduated with a BS in Chemistry and a minor in Physics and who started graduate school for computational chemistry at Princeton in Fall 2019; Madison Perchik, who graduated with a BS in chemistry and minors in Religious Studies and Spanish and who started medical school at the University of Tennessee in 2019, and Caroline Magee who graduated with a BS in chemistry and a minor in Religious Studies and is taking a gap year before applying to Dental School. All three women published a first-author manuscript on their computational chemistry research while undergraduates (the manuscript by Magee was accepted in her gap year and is in press); all three have presented their work

at the American Chemical Society Spring National Conferences in the COMP poster sessions, and all three presented their work at WATOC in Munich, Germany in 2017.

The latest data from the UNESCO Gender in Science-Women in Science study[1] shows that only 30% of STEM researchers worldwide are female. In 2018, Holloway and McGaughey studied gender data for the Computers in Chemistry Division (COMP) of the American Chemical Society (ACS) and found that the percentage that report as female plateaued at 18% in 2000[2]. Since members can opt out of reporting gender data, their best estimate of the actual percentage of female composition is about 25%. By contrast, the Medicinal Chemistry division of ACS has about 20% female membership[2]. Holloway and McGaughey suggest strategies for increasing the number of women in computational chemistry which include standard strategies such as building better gender balance in chemistry faculty and educating faculty members on unconscious bias, but also include more forward ideas such as *broadly communicating stories of women in science,* and putting women on panels, boards, speaker lists, *etc*. Indeed, research into increasing the number of women in STEM and making them feel welcomed supports the idea that outsized strategies must be employed to make the desired changes (see Cohoon for example[3]). Just as McGaughey *et al* accomplished in a 2019 paper[4], here we will communicate the stories of three undergraduate women who all found success while working in a computational chemistry lab, and we discuss the factors that lead them to feel accepted in this male-dominated field.

Professor Cafiero became Chair of the department of chemistry at Rhodes College for the 2013-2014 academic year, and since that time women have earned Bachelor's degrees in the department at a rate of 50% or higher in each year save for 2016-2017 (Table 1). During this time, the college itself has maintained an average distribution of about 55% women and 45% men. Thus the department has kept pace with the distribution at the College at large, and has, at times, exceeded the percentage of women that the college has. In his group, Professor Cafiero has had a 75%/25% split of women to men for the past two years (2017-2018 and 2018-2019). When he started at Rhodes College in 2004, his group was 100% male for the first two years—perhaps owing to a lack of experience with recruiting students who do not fall into the typical stereotype for theoretical/computational scientists—but it has been as high as 100% female for many of the years since.

**Table 1**. Total chemistry majors and % women in Chemistry at Rhodes College as taken from graduation rosters and in the Cafiero research group for each year from 2013 to the present.

| Academic Year | Graduated Chemistry Majors | # women | % women | Research Group Members | # women | % women |
|---|---|---|---|---|---|---|
| 2018-2019 | 24 | 12 | 50 | 16 | 12 | 75 |
| 2017-2018 | 15 | 11 | 73 | 18 | 14 | 78 |
| 2016-2017 | 15 | 5 | 33 | 12 | 10 | 83 |
| 2015-2016 | 19 | 11 | 58 | 10 | 9 | 90 |
| 2014-2015 | 16 | 11 | 69 | 6 | 6 | 100 |
| 2013-2014 | 17 | 9 | 53 | 6 | 6 | 100 |
| 2012-2013 | 20 | 5 | 25 | 4 | 4 | 100 |

**2. Recruitment of women and the role of peers/*Caroline Magee***

The work of Cohoon[3] specifically focuses on women in computing majors, but we believe their results may apply also to women who work in computational chemistry. They report that the single most effective strategy for increasing female participation in their field was to *actively recruit women*[3]. In a sort of "domino effect," they report that having more women in the field facilitates crucial peer mentoring; they report that having female peers is the most important coping mechanism that women in the field have[3]. They target women for recruitment in the first and second year and state that formalized application processes can discourage women who may have less prior experience with computing that a man of the same age and background[3]. Cohoon points out that strong faculty mentoring is what is needed to *retain* women once they are recruited ("*when her confidence failed her, she relied on her mentor's confidence in her*"[3]). Finally, they emphasize the need to communicate positive opinions of female's strengths and value those strengths[3]. Our lab has engaged in many of these practices over the past 15 years, particularly in how we recruit group members. The PI himself has actively recruited women who did well in his classes or otherwise showed a strong interest in chemistry or research as a career, but, more importantly, the students themselves have had a large role in recruiting and retaining students. In some cases, a student in the research group has urged a friend or fellow student to join the group, but more often they drive recruitment by being very visible.

The PI typically takes his group to three conferences per year: the MERCURY conference[5] for undergraduate computational chemistry students in the summer (the PI is a member of the MERCURY consortium), a regional conference in the Fall, and the national ACS conference in the Spring. The students also have opportunities to present their work at one additional local or regional conference each semester. Due to this continuous experience with preparing posters or talks and presenting their work, the students gain valuable experience with science communication and gain *confidence*. Because of this, the students in our group typically win presentation awards, which the PI promotes on the college's website as well as the college's Facebook and Instagram accounts. Even without earning awards, the PI usually publicizes the students who attended the conference regardless. *It is this publicity and exposure that drives most of the recruitment in our group.* The PI and students in the group have heard from both prospective college students and from current students at Rhodes that seeing women having this very visible attendance and success at national conferences has influenced their decision to attend Rhodes and inspired them to want to join this research group. The PI also goes beyond reporting conference attendance and participation and frequently submits students from the group to be profiled in a more broad sense on the college's website and social media. Thus, it is the accomplishments of other women in the group that influence prospective group members to seek out Professor Cafiero about joining the group. Recruitment in this group is accomplished via two routes: about half of new members are invited to join by Professor Cafiero after performing well in his classes and about half approach him directly. Most of the new members, regardless of recruiting technique, cite the visibility and accomplishment of current group members in their desire to join.

> *Though I have always been a curious and determined student, even before college I always sought that extra support and encouragement from a mentor or my peers to boost my*

*confidence. Having a strong group of women and a mentor that encouraged us all to maximize our education is what I will never forget as an undergraduate researcher. Being asked to join a research group and learning how to tie in knowledge from my chemistry major and computational chemistry research to the "outside world" was such pivotal point in my undergraduate career because of. My relationship with Dr. Cafiero's research group was started before I started school at Rhodes College and still continues to this day.*

*During my senior year of high school I visited campus for accepted students day; during that visit I wanted to take a look around the chemistry building to see where my future "home" would be. I heard laughs and chatter from down the hall and decided to walk towards it to see what all the excitement was about. I peeked my head around the corner and saw a group of undergraduate women in a room working on computers and while chatting with Dr. Cafiero. He waved from inside the room to say hello and walked out to introduce himself. Little did I know that conversation with Dr. Cafiero would lead four years working in the research group.*

*Later that summer before my first year at Rhodes, I attended summer orientation and was assigned to small group advising in the Chemistry department with my future mentor, Dr. Cafiero, and a few other new students. As we were signing up for classes, a group of older undergraduate women from his research group came in to answer any questions we had about choosing class and college in general. From the start, they facilitated a discussion as peer-mentors that helped guide us to choose classes that were a good fit. The support and encouragement that was coming from each of those women made me confident in the decisions that I made. The environment that they created was welcoming and made me comfortable asking them questions and made me excited to explore all the possibilities of my college education. I was quickly able to trust them because they gave so much advice at a professional level and told me their honest opinions. Seeing a large group of women collectively helping future students wanting to pursue a career in science was very encouraging. They made me aspire to be like them and follow a similar path leading to success.*

*After discussing it with Prof. Cafiero that summer, I agreed to do research with him. I was assigned a peer-mentor that has been in the group for a few years and would teach me all the lab protocols I needed to know. Going into the research lab my first week of school I was nervous that I did not have the knowledge to conduct research, but by having my new peer-mentor and Dr. Cafiero nearby I was able to pick up quickly. The women in the group were always there to answer questions that I had and even offered their phone number in case I needed anything. During my first semester, my peer-mentor who I had been assisting wanted me to present her research with her. This led to me attending my first Research Conference during my first semester of school. Having presented the research with her made me more confident in my ability to communicate science. As a celebration for our hard work and accomplishments at that and every subsequent conference, Dr. Cafiero sends a picture of our research group and a summary of our accomplishments to the College's*

*communications office for them to distribute widely. This creates a positive image to our campus of women in computational chemistry.*

*Being surrounded by this strong group of women and Dr. Cafiero has helped mold me into the person who I am today. I am more confident and comfortable presenting my research in both poster oral presentations. It became natural to answer questions from graduate students and faculty members about my research during conferences because of how supportive and helpful my peer-mentors were. They were able to guide me and teach me what to say and how to explain it. A couple of years later, I was given my own first-year student to educate and mentor on the skills to help her succeed just like my mentors helped me. All of the women in our research group have a common goal to understand computational chemistry and take it to the next level by sharing our knowledge and passion for chemistry. Our computational chemistry research group created relationships that fed off each other to form a strong network of hardworking and intelligent women.*

*-Caroline Magee, Class of 2019*

**3. Support for women after recruitment and the role of mentors/*Madison Perchik***

Fox *et al* report the characteristics of successful programs for undergraduate women in science[6]. Among their points, they state that programs that successfully support women see female representation as a *faculty issue* (for example, unconscious bias among faculty such as "*weed-out culture*") and recognize the lack of pipeline support after recruiting women. They emphasize that successful programs create equitable environments including *academic, professional and social aspects*[6]. These issues often come down to the mentors or potential mentors that are available. Much work has been done on how mentors can help and retain women in STEM. A study by Russell *et al* published in *Science* shows that success for women (and minorities) *does not* depend on having a woman or minority mentor; rather the best mentors for women (or students in general) are those who are enthusiastic and bring good interpersonal and organization skills to bear, apart from just research skills[7]. They do point out that the better outcomes for students are achieved when students have two mentors from two different demographics[7]. An older study by Hammick and Acker[8] shows that outcomes for women such as publications *do not* depend on the gender of their supervisor, though professional development may. In this study male mentors are found to have more distant relationships with female students and were much less likely to discuss personal matters with female students. These male mentors saw the relationship with the student as task/knowledge oriented rather than person oriented. Men were also more likely to blame failures on students[8]. These issues for male mentors can become outsized problems, as a 2000 study showed that students want advisors who available, patient and enthusiastic[9].

Professor Cafiero has always seen the relationship between himself and the students in his group as the most important factor in research productivity. A study by Settles, *et al* discuss the fact that a positive climate and positive treatment by a supervisor and peers leads to higher satisfaction and productivity among women in academia[10]. By the same token, social isolation among women leads to lower productivity[10]. As a male, Professor Cafiero has taken care to create environments that support

women in particular. Among these efforts has been the creation of a strong group identity and opportunities for socialization among group members. He holds social events to celebrate group member birthdays as well as the end of the semester. These social events are usually held in the daytime, are often staged in the research lab, and are not "mandatory." During travel for research conferences Professor Cafiero plans all-day agenda of activities for the group to do together; this simultaneously builds group camaraderie and also helps students who may feel left out or that they "don't belong" if the group does not have planned activities. Finally, Professor Cafiero has always tried to give each student the amount of attention and mentoring that is right for them. Some students seek advice on just research; some seek advice on research and other classes; some seek advice on research, classes, and their future career paths; and some seek advice on all of these things and personal matters. By being available to meet a student's needs at the level that is comfortable for the student, Professor Cafiero tries to create an environment that is welcoming for all, and he finds that many students progress through these levels of support at their own pace during their time in college.

> *Mentorship has been and continues to be a major driver in my ability to succeed. I hoped that choosing a small college would allow me to cultivate close relationships with my professors as I had during my previous schooling. This decision is one that I will always be grateful for, as the mentorship I received in college has shaped my life in more ways than I could have ever hoped for. After I was recruited into the research group during my first year of college, I was shown unwavering patience and enthusiasm by Dr. Cafiero, my official mentor, and by the other members of the group. It was obvious that Dr. Cafiero had worked hard to create a culture of acceptance and collaboration in his research group long before I got there. He empowered the members to interweave our projects, to bounce ideas off of each other, and to share our mistakes and successes. I feel so fortunate to have been a part of this type of environment, as I feel it is sometimes undervalued in the scientific community. Since I have now personally seen how beneficial this collaborative, supportive environment is, I will do everything I can to implement these ideals in any group setting that I find myself in.*
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> *It is important to note that this type of environment must be intentional. I believe that it starts with a conscious effort by the mentor to create and maintain this type of environment. From the very beginning of my time in the research group, Dr. Cafiero put just as much effort into learning about me as a person as he did teaching me the details of our research project. He became my biggest supporter and someone that I knew that I could go to with every frustration, set back, or celebration in all aspects of my life. Because he knew me, he knew the best ways to explain complex topics to me or how to give the most appropriate advice. Because I got to know him and my fellow research members beyond our projects, my passion for our research did not only come from my personal desire to ask questions and pursue possible answers. My passion for our research also came from the desire to push forward an initiative set by someone who I admired and to continue the work of the many talented people around me and those who came before me.*
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> *In my opinion, one of the pillars of successful mentorship is allowing a safe space for error and growth. Again, this is not a passive process on the mentor's part. Conscious effort must be*

*employed to create this safe space, especially if one is working with women. As a woman, we are socialized to be meek and to second-guess ourselves, especially in male-dominated settings. Dr. Cafiero counteracted this social norm from the very beginning of our time together through his commitment to accessibility and his ability to always use errors as teaching moments instead of opportunities to criticize. His accessibility, whether it be through text, email, office hours, research hours, etc., allowed me to always feel comfortable asking questions. His encouraging and teaching-centered attitude allowed me to make mistakes often, learn quickly, and to explore my scientific creativity. When it came time for me to start my independent study, I knew that each idea that I pursued would be met with support and helpful suggestions from my mentor instead of being ignored or immediately shot down. The impact of Dr. Cafiero's mentorship on me is life-long. I am committed to mentoring young professionals in my field as soon as I get the opportunity.*

*-Madison Perchik, Class of 2019*

**4. Obstacles women face in attaining careers in science research/*Rebecca Evans***

The lack of women in research science has prompted many studies into what obstacles they face in transitioning from girls who are good at math and science, to women who major in STEM in college, to women in research. A study from 2004 focused on the effect of undergraduate research on career goals of science students [11]. While 58% of the respondents were women, only 10% of those women planned to continue a Ph.D. in science after earning their undergraduate degree, compared with 22% of men who planned to do so[11]. A recent study of data on people who were in high school in the UK in the 1970's shows that women in single sex schooling in elementary school and/or high school were largely able to overcome some of the obstacles commonly faced by women. These women were less likely to see themselves as below average in science and math, they scored better on standardized exams, there were more likely to study in male-dominated fields, and they gained higher wages later in life[12]. A recent study by Yang *et al* shows that centrality in a network of well-connected, communicative women has an outsized effect on women's placement in leadership positions when compared with exam scores, GPA, work experience and sociability[13]. It may be that the networks developed during single-sex schooling help with maintaining and establishing these networks later in life.

One of the major obstacles that can hold women back is their access or lack of access to mentors. Even for women who have mentors, these mentors can have lowered expectations for women compared to men and can purposefully or unconsciously exclude women from social networks[14]. It is in cases such as these that female peer network support is especially important[11,12,14]. The women in Professor Cafiero's group obviously have him as a resource to help overcome these obstacles, but, most importantly, they have the legacy and advice of the women who have come before them. As mentioned in the abstract, female alums of the group include M.D.s, scientists, entrepreneurs, teachers, and other health professionals. Professor Cafiero works to make sure that all of his group members are connected with alums of the group for advice on how to attain their goals using the experience that they have from the research group.

*I clearly remember the day in my junior year that Dr. Cafiero suggested I apply to Princeton for graduate school. I asked him if he thought I could actually get in; to me it seemed like an impossibility. Had it not been for Dr. Cafiero's immediate and sustained support, I never would have applied to Princeton. So, the first person I called when I got into Princeton University's graduate program was Dr. Cafiero. He picked up the phone, despite being in the middle of teaching a lab. Telling Dr. Cafiero made my success feel concrete.*

*I met Dr. Cafiero on the first day of new student orientation when he was assigned as my advisor. I was a first-generation college student, living 1,000 miles from home, and--despite my best efforts--I had no idea what I was doing. I knew that I wanted to study chemistry and possibly work in the pharmaceutical industry, but my knowledge of collegiate life ended there. After discussing my interests and future plans, Dr. Cafiero invited me to join his research group as early as my first semester at Rhodes. At the time, I was so unsure of myself that I was sure the invitation was ingenuine, and it took me until the end of my first year to approach Dr. Cafiero and ask about his offer. It was not until he introduced me to the lab and I met all the other women that I realized they were just like me. Seeing this group of smart women and knowing I fit in was what helped me finally accept Dr. Cafiero's offer. Once I joined the group, I was assigned to be mentored by one of the senior members of the group, Katie. I remembered viewing Katie as a chemistry superstar. She had gone to conferences and published two papers. When she went off to graduate school the next year, she became an example of who I wanted to be in three years. During my senior year I even used her personal essay as inspiration to write my own, and when I was invited to visit her graduate school, she arranged to meet with me and made sure I felt comfortable and answered the millions of questions I had. Having that role model to look up to throughout my undergraduate education was invaluable.*

*In Dr. Cafiero's lab I immediately fell in love with the process of research. His mentorship and the support of my fellow lab mates was just the cherry on top. I presented my first poster at an American Chemical Society national meeting a year after I joined the lab. Over the course of my undergraduate career, I gave 13 research presentations, two of which were at international conferences. On more than one occasion, I received condescending remarks about my research. In one instance I had a researcher seek me out to "mansplain" my own research to me. Although discouraging, I received overwhelming support from the women around me and Dr. Cafiero, ensuring me that although being a minority in the field I had earned my knowledge and my place in the community. I found presenting my research only emboldened me to give more presentations to defend my work.*

*Many of the conferences I attended as an undergraduate had primarily male participants; this proportion was further skewed at field specific conferences. The first conference I attended on my own was an international computational chemistry symposium where I was one of four women in a room of 100 men. Not being able to relate to a majority of the other attendees made it difficult to feel like I belonged in the room. Instances like these can be dissuading to young women who may feel unwelcomed by the members of their field. In*

*response, I have tried to use my passion for representation to help other young women in applying for graduate programs in chemistry and the natural sciences. I have helped them the same way Katie helped me, by giving them everything from essay edits and resume templates to outfit advice. I want to help to increase women's presence and confidence in a field where they may not receive the necessary support.*

*I was lucky, and I had the support that I needed from Dr. Cafiero and the rest of the lab. When I asked Dr. Cafiero if I could publish an article on my research, he gave me the resources and support to do so; when I needed help navigating the graduate admissions process, he was always available to read over application materials; and when I was unsure of my research or abilities or myself, I had a supportive mentor in Dr. Cafiero in addition to a group of intelligent, science-minded women in my own research group to whom I could reach out. When I arrived at Princeton University, I wrote myself a note that I turn to often when I feel unsure or underqualified: "You are incredibly smart and insightful, if you weren't you wouldn't be here." This is the sentiment that I think more women should tell themselves, but more importantly, it is what they should hear from others.*

*-Rebecca Evans, Class of 201*9

**5. Best practices**

The experiences of these three students—and of the group in general—can be summarized as the suggested best practices below.

I. *It takes women to recruit women.* We believe that the best motivation for a woman to join a research group and see herself as being successful there is to see other successful women there. A woman working in isolation from other women faces more obstacles than women working together.

II. *Promote, promote, promote!* Women are less likely to speak out about their accomplishments, and so it is the responsibility of the advisor to do all they can to make these women and their accomplishments as visible as possible on campus and in the field.

III. *Support the whole student.* Women in male-dominated fields have different mentoring needs than males, not the least of which is personal mentoring (as opposed to professional). Meet each woman at the place where they need support and be there for them. Some will need more support than others, but all will need some level of help. This point is especially important for male advisors who are traditionally reluctant to go beyond professional mentoring with women.

IV. *Give them opportunities.* In order to get to the next step in their career paths, women have to show a legacy of accomplishment—in some cases moreso than their male peers. Make sure that you send them to conferences and workshops, that you introduce them to people in the field, and that you give them a chance

to publish if at all possible. Advocate for them for opportunities, awards, jobs and graduate school admissions.

As a result of implementing these best practices, Professor Cafiero's research group has benefitted from having a large female presence. Notably, having a strong female peer-support system improves mental health of students[3]. This in turn improves productivity. The students in Professor Cafiero's group present their work at conferences at least once per year, and sometimes four times per year. Professor Cafiero's group produces 1.3 peer-reviewed manuscripts per year on average, which is more than double the average for physical science faculty members at primarily undergraduate institutions. As can be seen in the stories above, strong peer-mentoring helps with recruiting, retention and prodictivity. In short, supporting more women means we get *more science!*

**6. Other types of diversity**

While Professor Cafiero and his group have a history of strongly supporting women in a predominately male field, work remains on increasing support for other underrepresented groups. While his research group has included Hispanic, lesbian, gay, and bisexual students over the past fifteen years, it has notably lacked black and other minority students, and, in particular, black or Hispanic male students. Part of this deficiency has to do with the demographics of the college and the major, but part is due to failures in recruitment.

While each minority has their own challenges to overcome in the pursuit of a career in science, the techniques described above and already in use to recruit and retain women can be similarly adapted and used to recruit and retain other under-represented minorities. From intentional recruitment, to a strong network of peer-mentors, to sensitive faculty mentoring, and to providing the resources to reach career goals, all of these tools can be levied to promote other under-represented groups in our field as we have done with women, and we look forward to making progress towards this goal.

The MERCURY consortium[5] has a long tradition of supporting women and other under-represented minorities[15]. This group of computational chemists at primarily undergraduate institutions has had continuous funding from the National Science Foundation for almost twenty years. Since 2001, the over-one-thousand students who have worked with faculty in the MERCURY consortium have included 75% who are underrepresented in chemistry, either female or students of color. The close mentoring ties among the faculty in the consortium ensure that best practices for recruiting and retaining women and minority students are passed along.

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